

DEPHASING AND RENORMALIZATION IN QUANTUM TWO-LEVEL SYSTEMS

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Abstract.

Motivated by fundamental questions about the loss of phase coherence at low temperature we consider relaxation, dephasing and renormalization effects in quantum two-level systems which are coupled to a dissipative environment. We observe that experimental conditions, e.g., details of the initial state preparation, determine to which extent the environment leads to dephasing or to renormalization effects. We analyze an exactly solvable limit where the relation between both can be demonstrated explicitly. We also study the effects of dephasing and renormalization on response functions.

1. Introduction

The dynamics of quantum two-level systems has always been at the focus of interest, but recently attracted increased attention because of the prospects of quantum state engineering and related low-temperature experiments. A crucial requirement for many of these concepts is the preservation of phase coherence in the presence of a noisy environment. Typically one lacks a detailed microscopic description of the noise source, but frequently it is sufficient to model the environment by a bath of harmonic oscillators, with frequency spectrum adjusted to reproduce the observed power spectrum.

The resulting ‘spin-boson’ models have been studied in the literature, in particular the one with bilinear coupling and ‘Ohmic’ spectrum, but spin-boson models with different power spectra appear equally interesting in view of several experiments. In this article we, therefore, analyze spin-boson model with general power spectra with respect to relaxation, dephasing and renormalization processes at low temperatures. We study the dephasing of nonequilibrium initial states. We show how the state preparation affects the effective high-frequency cut-off and separates renormalization from dephasing effects. We also demonstrate how dephasing processes influence low-temperature linear response and correlation functions.

2. Spin-boson model

In this section we review the theory and properties of spin-boson models, which have been studied extensively before (see the reviews [4, 11]). A quantum two-level system is modeled by a spin degree of freedom in a magnetic field. It is coupled linearly to an oscillator bath representing the environment. The total Hamiltonian is

$$\mathcal{H} = \mathcal{H}_{\text{ctrl}} + \sigma_z \sum_j c_j (a_j + a_j^\dagger) + \mathcal{H}_b, \quad (1)$$

where the controlled part is $\mathcal{H}_{\text{ctrl}} = -\frac{1}{2}B_z \sigma_z - \frac{1}{2}B_x \sigma_x = -\frac{1}{2}\Delta E (\cos \theta \sigma_z + \sin \theta \sigma_x)$, the oscillator bath is described by $\mathcal{H}_b = \sum_j \hbar \omega_j a_j^\dagger a_j$, and the bath ‘force’ operator $X = \sum_j c_j (a_j + a_j^\dagger)$ is assumed to couple linearly to σ_z . For later convenience $\mathcal{H}_{\text{ctrl}}$ has also been written in terms of a mixing angle $\theta = \tan^{-1}(B_x/B_z)$, depending on the direction of the magnetic field, and the energy splitting of the eigenstates, $\Delta E = \sqrt{B_x^2 + B_z^2}$.

In thermal equilibrium the Fourier transform of the symmetrized correlation function of the force operator is given by

$$S_X(\omega) \equiv \langle [X(t), X(t')]_+ \rangle_\omega = 2\hbar J(\omega) \coth \frac{\hbar \omega}{2k_B T}. \quad (2)$$

Here the bath spectral density has been introduced, defined by $J(\omega) \equiv \frac{\pi}{\hbar} \sum_j c_j^2 \delta(\omega - \omega_j)$. At low frequencies it typically has a power-law form up to a high-frequency cut-off ω_c ,

$$J(\omega) = \frac{\pi}{2} \hbar \alpha \omega_0^{1-s} \omega^s \Theta(\omega_c - \omega). \quad (3)$$

Generally one distinguishes Ohmic ($s = 1$), sub-Ohmic ($s < 1$), and super-Ohmic ($s > 1$) spectra. In Eq. (3) an additional frequency scale ω_0 has been introduced. Since it appears only in the combination $\alpha \omega_0^{1-s}$ it is arbitrary

and in Ref. [4] has been chosen equal to the high-frequency cut-off. Here we prefer to distinguish both frequencies, since the cut-off ω_c will play an important role in what follows.

The spin-boson model has been studied mostly for the case where an Ohmic bath is coupled linearly to the spin. One reason is that linear damping, proportional to the velocity, is encountered frequently in real systems. Another is that suitable systems with Ohmic damping show a quantum phase transition at a critical strength of the dissipation, $\alpha_{\text{cr}} \sim 1$. On the other hand, in the context of quantum-state engineering we should concentrate on systems with weak damping, but allow for general spectra of the fluctuations.

Spin-boson models with sub-Ohmic damping ($0 < s < 1$) have been considered earlier [4, 11] but did not attract much attention. It was argued that sub-Ohmic dissipation would totally suppress coherence, transitions between the states of the two-level system would happen only at finite temperatures and would be incoherent. At zero temperature the system should be localized in one of the eigenstates of σ_z , since the bath renormalizes the off-diagonal part of the Hamiltonian B_x to zero. This scenario is correct for intermediate to strong damping. It is, however, not correct for weak damping. Indeed the ‘NIBA’ approximation developed in Ref. [4] fails in the weak-coupling limit for transverse noise, while a more accurate renormalization procedure [3] predicts damped coherent behavior. In the context of quantum-state engineering we are interested in precisely this *coherent sub-Ohmic* regime. We will demonstrate a simple criterion which allows to define a border between coherent and incoherent regimes.

A further reason to study the sub-Ohmic case is that it allows us to mimic the universally observed $1/f$ noise. For instance, a bath with $s = 0$ and $J(\omega) = (\pi/2)\alpha\hbar\omega_0$ produces at low frequencies, $\hbar\omega \ll k_B T$, a $1/f$ noise spectrum $S_X(\omega) = E_{1/f}^2/|\omega|$ with $E_{1/f}^2 = 2\pi\alpha\hbar\omega_0 k_B T$. Since frequently nonequilibrium sources are responsible for the $1/f$ noise, the temperature here should be regarded as a fitting parameter rather than a thermodynamic quantity.

Below we will also consider the super-Ohmic case ($s > 1$) as it allows us to study renormalization effects clearly.

3. Relaxation and dephasing

We first consider the Ohmic case in the weak damping regime, $\alpha \ll 1$. Still we distinguish two regimes: the ‘Hamiltonian-dominated’ regime, which is realized when ΔE is large enough, and the ‘noise-dominated’ regime, which is realized, e.g., at degeneracy points where $\Delta E \rightarrow 0$. The exact border between both regimes will be specified below.

In the Hamiltonian-dominated regime it is natural to describe the evolution of the system in the eigenstates of $\mathcal{H}_{\text{ctrl}}$, which are

$$|0\rangle = \cos \frac{\theta}{2} |\uparrow\rangle + \sin \frac{\theta}{2} |\downarrow\rangle \quad \text{and} \quad |1\rangle = -\sin \frac{\theta}{2} |\uparrow\rangle + \cos \frac{\theta}{2} |\downarrow\rangle . \quad (4)$$

Denoting by τ_x and τ_z the Pauli matrices in the eigenbasis, we have

$$\mathcal{H} = -\frac{1}{2}\Delta E \tau_z + (\sin \theta \tau_x + \cos \theta \tau_z) X + \mathcal{H}_b . \quad (5)$$

Two different time scales describe the evolution in the spin-boson model. The first, the dephasing time scale τ_φ , characterizes the decay of the off-diagonal elements of the qubit's reduced density matrix $\hat{\rho}(t)$ in the preferred eigenbasis (4), or, equivalently of the expectation values of the operators $\tau_\pm \equiv (1/2)(\tau_x \pm i\tau_y)$. Frequently dephasing processes lead to an exponential long-time dependence,

$$\langle \tau_\pm(t) \rangle \equiv \text{tr} [\tau_\pm \hat{\rho}(t)] \propto \langle \tau_\pm(0) \rangle e^{\mp i\Delta E t/\hbar} e^{-t/\tau_\varphi} , \quad (6)$$

but other decay laws occur as well and will be discussed below. The second, the relaxation time scale τ_{relax} , characterizes how diagonal entries tend to their equilibrium values,

$$\langle \tau_z(t) \rangle - \langle \tau_z(\infty) \rangle \propto e^{-t/\tau_{\text{relax}}} , \quad (7)$$

where $\langle \tau_z(\infty) \rangle = \tanh(\Delta E/2k_B T)$.

In Refs. [4, 11] the dephasing and relaxation times were evaluated in a path-integral technique. In the regime $\alpha \ll 1$ it is easier to employ the perturbative (diagrammatic) technique developed in Ref. [9] and the standard Bloch-Redfield approximation. The rates are

$$\Gamma_{\text{relax}} \equiv \tau_{\text{relax}}^{-1} = \frac{1}{\hbar^2} \sin^2 \theta S_X(\omega = \Delta E/\hbar) , \quad (8)$$

$$\Gamma_\varphi \equiv \tau_\varphi^{-1} = \frac{1}{2} \Gamma_{\text{relax}} + \frac{1}{\hbar^2} \cos^2 \theta S_X(\omega = 0) , \quad (9)$$

where $S_X(\omega) = \pi \alpha \hbar^2 \omega \coth(\hbar \omega/2k_B T)$. We observe that only the ‘transverse’ part of the fluctuating field X , coupling to τ_x and proportional to $\sin \theta$, induces transitions between the eigenstates (4) of the unperturbed system. Thus the relaxation rate¹ (8) is proportional to $\sin^2 \theta$. The ‘longitudinal’ part of the coupling of X to τ_z , which is proportional to $\cos \theta$, does

¹The equilibration is due to two processes, excitation $|0\rangle \rightarrow |1\rangle$ and relaxation $|1\rangle \rightarrow |0\rangle$, with rates $\Gamma_{+/-} \propto \langle X(t)X(t') \rangle_{\omega=\pm\Delta E/\hbar}$. Both rates are related by a detailed balance condition, and the equilibrium value $\langle \tau_z(\infty) \rangle$ depends on both. On the other hand, Γ_{relax} is determined by the sum of both rates, i.e., the symmetrized noise power spectrum S_X .

not induce relaxation processes. It does, however, contribute to dephasing since it leads to fluctuations of the eigenenergies and, thus, to a random relative phase between the two eigenstates. This is the origin of the ‘pure’ dephasing contribution to Eq. (9), which is proportional to $\cos^2 \theta$. We rewrite Eq. (9) as $\Gamma_\varphi = \frac{1}{2}\Gamma_{\text{relax}} + \cos^2 \theta \Gamma_\varphi^*$, where $\Gamma_\varphi^* = S_X(\omega = 0)/\hbar^2 = 2\pi\alpha k_B T/\hbar$ is the pure dephasing rate.

The pure dephasing rate Γ_φ^* characterizes the strength of the dissipative part of the Hamiltonian, while ΔE characterizes the coherent part. The Hamiltonian-dominated regime is realized when $\Delta E \gg \Gamma_\varphi^*$, while the noise-dominated regime is realized in the opposite case.

In the noise-dominated regime, $\Delta E \ll \Gamma_\varphi^*$, the coupling to the bath is the dominant part of the total Hamiltonian. Therefore, it is more convenient to discuss the problem in the eigenbasis of the observable σ_z to which the bath is coupled. The spin can tunnel incoherently between the two eigenstates of σ_z . One can again employ the perturbative analysis [9], but use directly the Markov instead of the Bloch-Redfield approximation. The resulting rates are given by

$$\begin{aligned}\Gamma_{\text{relax}} &= B_x^2/\Gamma_\varphi^* = B_x^2/(2\pi\hbar\alpha k_B T) \\ \Gamma_\varphi &= \Gamma_\varphi^* = 2\pi\hbar\alpha k_B T.\end{aligned}\tag{10}$$

In this regime the dephasing is much faster than the relaxation. In fact, as a function of the coupling strength α the dephasing and relaxation rates evolve in opposite directions. The α -dependence of the relaxation rate is an indication of the Zeno (watchdog) effect [2]: the environment frequently ‘observes’ the state of the spin, thus preventing it from tunneling.

4. Longitudinal coupling, exact solution for factorized initial conditions

The last forms of Eqs. (8) and (9) express the two rates in terms of the noise power spectrum at the relevant frequencies. These are the level spacing of the two-state system and zero frequency, respectively. The expressions apply in the weak-coupling limit for spectra which are regular at these frequencies. For the relaxation rate (8) the generalization to sub- and super-Ohmic cases merely requires substituting the relevant $S_X(\omega = \Delta E/\hbar)$. However, this does not work for the pure dephasing contribution. Indeed $S_X(\omega = 0)$ is infinite in the sub-Ohmic regime, while it vanishes for the super-Ohmic case and the Ohmic case at $T = 0$. As we will see this does not imply infinitely fast or slow dephasing in these cases. To analyze these cases we study the exactly soluble model of longitudinal coupling, $\theta = 0$.

Dephasing processes are contained in the time evolution of the quantity $\langle\tau_+(t)\rangle$ obtained after tracing out the bath. This quantity can be evaluated

analytically for $\theta = 0$ (when $\tau_+ = \sigma_+$) for an initial state which is described by a factorized density matrix $\hat{\rho}(t = 0) = \hat{\rho}_{\text{spin}} \otimes \hat{\rho}_{\text{bath}}$ (which implies that the two-level system and bath are initially disentangled). In this case the Hamiltonian $\mathcal{H} = -\frac{1}{2}\Delta E \sigma_z + \sigma_z X + \mathcal{H}_b$ is diagonalized by a unitary transformation by $U \equiv \exp(-i\sigma_z \Phi/2)$ where the bath operator Φ is defined as

$$\Phi \equiv i \sum_j \frac{2c_j}{\hbar\omega_j} (a_j^\dagger - a_j). \quad (11)$$

The ‘polaron transformation’ yields $\tilde{\mathcal{H}} = U\mathcal{H}U^{-1} = -\frac{1}{2}\Delta E \sigma_z + \mathcal{H}_b$. It has a clear physical meaning: the oscillators are shifted in a direction depending on the state of the spin. Next we observe that the operator σ_+ is transformed as $\tilde{\sigma}_+ = U\sigma_+U^{-1} = e^{-i\Phi}\sigma_+$, and the observable of interest can be expressed as

$$\langle \sigma_+(t) \rangle = \text{Tr} [\hat{\rho}(t=0)\sigma_+(t)] = \text{Tr} [U\hat{\rho}(t=0)U^{-1}e^{-i\Phi(t)}\sigma_+] . \quad (12)$$

The time evolution of $\Phi(t) = e^{i\mathcal{H}_b t}\Phi e^{-i\mathcal{H}_b t}$ is governed by the bare bath Hamiltonian. After some algebra, using the fact that the initial density matrix is factorized, we obtain $\langle \sigma_+(t) \rangle \equiv \mathcal{P}(t) e^{-i\Delta E t} \langle \sigma_+(0) \rangle$ where

$$\mathcal{P}(t) = \text{Tr} \left[e^{i\Phi(0)/2} e^{-i\Phi(t)} e^{i\Phi(0)/2} \hat{\rho}_{\text{bath}} \right] . \quad (13)$$

The expression (13) applies for any initial state of the bath as long as it is factorized from the spin. In particular, we can assume that the spin was initially (for $t \leq 0$) kept in the state $|\uparrow\rangle$ and the bath had relaxed to the thermal equilibrium distribution for this spin value: $\hat{\rho}_{\text{bath}} = \hat{\rho}_\uparrow \equiv Z_\uparrow^{-1} e^{-\beta\mathcal{H}_\uparrow}$, where $\mathcal{H}_\uparrow = \mathcal{H}_b + \sum_j c_j (a_j + a_j^\dagger)$. In this case we can rewrite the density matrix as $\hat{\rho}_{\text{bath}} = e^{i\Phi/2} \hat{\rho}_b e^{-i\Phi/2}$, where the density matrix of the decoupled bath is given by $\hat{\rho}_b \equiv Z_b^{-1} e^{-\beta\mathcal{H}_b}$, and the function $\mathcal{P}(t)$ reduces to

$$\mathcal{P}(t) \rightarrow P(t) \equiv \text{Tr} \left(e^{-i\Phi(t)} e^{i\Phi} \hat{\rho}_b \right) . \quad (14)$$

This expression (with Fourier transform $P(E)$) has been studied extensively in the literature [4, 8, 7, 6, 1]. It can be expressed as $P(t) = \exp K(t)$, where

$$K(t) = \frac{4}{\pi\hbar} \int_0^\infty d\omega \frac{J(\omega)}{\omega^2} \left[\coth \left(\frac{\hbar\omega}{2k_B T} \right) (\cos \omega t - 1) - i \sin \omega t \right] . \quad (15)$$

For an Ohmic bath at non-zero temperature and not too short times, $t > \hbar/k_B T$, it reduces to $\text{Re} K(t) \approx -S_X(\omega = 0)t/\hbar^2 = -2\pi \alpha k_B T t/\hbar$, consistent with Eq. (9) in the limit $\theta = 0$.

For $1/\omega_c < t < \hbar/k_B T$, and thus for all times at $T = 0$, one still finds a decay of $\langle \sigma_+(t) \rangle$ governed by $\text{Re } K(t) \approx -2 \alpha \ln(\omega_c t)$, which implies a power-law decay

$$\langle \sigma_+(t) \rangle = (\omega_c t)^{-2\alpha} e^{-i\Delta E t/\hbar} \langle \sigma_+(0) \rangle. \quad (16)$$

Thus even at $T = 0$, when $S_X(\omega = 0) = 0$, the off-diagonal elements of the density matrix decay in time. All oscillators up to the high-frequency cut-off ω_c contribute to this decay. The physical meaning of this result will be discussed later. We can also define a cross-over temperature T^* below which the power-law decay dominates over the subsequent exponential one. A criterion is that at $t = \hbar/k_B T^*$ the short-time power-law decay has reduced the off-diagonal components already substantially, i.e. $\langle \sigma_+(\hbar/k_B T^*) \rangle = 1/e$. This happens at the temperature $kT^* = \hbar\omega_c \exp(-1/2\alpha)$. Thus the dephasing rate is $\Gamma_\varphi^* = k_B T^*/\hbar$ for $T < T^*$ and $\Gamma_\varphi^* = 2\pi\alpha k_B T/\hbar$ for $\alpha T > T^*$.

For a sub-Ohmic bath with $0 < s < 1$ due to the high density of low-frequency oscillators exponential dephasing is observed even for short times, $|\langle \sigma_+(t) \rangle| \propto \exp[-\alpha(\omega_0 t)^{1-s}]$ for $t < \hbar/k_B T$, as well as for longer times, $|\langle \sigma_+(t) \rangle| \propto \exp[-\alpha T t (\omega_0 t)^{1-s}]$ for $t > \hbar/k_B T$. In the exponents of the short- and long-time decay laws we have omitted factors which are of order one, except if s is close to either 1 or 0, in which case a more careful treatment is required. The dephasing rates resulting from the decay laws are $\Gamma_\varphi^* \propto T^* = \alpha^{1/(1-s)} \omega_0$ (cf. Ref. [10]) for $T < T^*$ and $\Gamma_\varphi^* \propto (\alpha T/\omega_0)^{1/(2-s)} \omega_0$ for $T > T^*$. Again the crossover temperature T^* marks the boundary between the regimes where either the initial, temperature-independent decay or the subsequent decay at $t > \hbar/k_B T$ is more important.

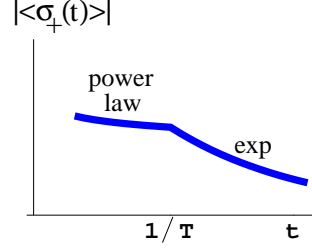
These results allow us to further clarify the question of coherent vs. incoherent behavior in the sub-Ohmic regime. It is known from earlier work [4, 11] that the dynamics of the spin is incoherent even at $T = 0$ if $\Delta E \ll \alpha^{1/(1-s)} \hbar \omega_0$ (only the transverse case $\theta = \pi/2$ was considered). This condition implies $\Delta E \ll \Gamma_\varphi^*$, i.e., it marks the noise-dominated regime. We are mostly interested in the opposite, Hamiltonian-dominated regime, $\Delta E \gg \hbar \Gamma_\varphi^*$. The NIBA approximation used in Ref. [4] fails in this limit, while a more accurate RG study [3] predicts damped coherent behavior.

Finally we discuss the super-Ohmic regime, $s > 1$. In this case, within a short time of order ω_c^{-1} , the exponent $\text{Re } K(t)$ increases to a finite value $\text{Re } K(\infty) = -\alpha(\omega_c/\omega_0)^{s-1}$ and then remains constant for $\omega_c^{-1} < t < \hbar/k_B T$ (we again omit factors of order one and note that the limit $s \rightarrow 1$ requires more care). This implies an initial reduction of the off-diagonal element $|\langle \sigma_+(t) \rangle|$ followed by a saturation at $|\langle \sigma_+(t) \rangle| \propto \exp[-\alpha(\omega_c/\omega_0)^{s-1}]$. For $t > \hbar/k_B T$ an exponential decay develops, $|\langle \sigma_+(t) \rangle| \propto \exp[-\alpha T t (\omega_0 t)^{1-s}]$, but only if $s < 2$. This decay is always dominant and, thus, there is no

TABLE 1. Decay of $|\langle\sigma_+(t)\rangle|$ in time for different bath spectra.

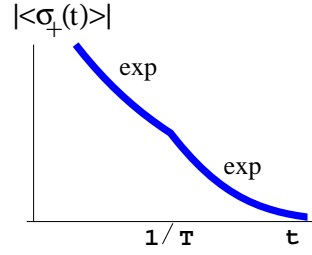
- Ohmic: $J(\omega) = \frac{\pi}{2}\alpha\omega\Theta(\omega_c - \omega)$:

$$\begin{array}{ll} \text{for } \omega_c^{-1} \ll t \ll T^{-1} & |\langle\sigma_+(t)\rangle| \approx (\omega_c t)^{-2\alpha} \\ \text{for } t \gg T^{-1} & |\langle\sigma_+(t)\rangle| \approx e^{-2\pi\alpha T t} \end{array}$$



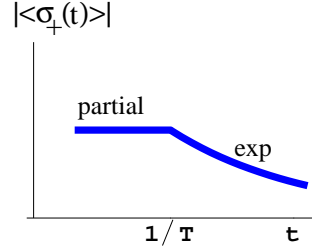
- Sub-Ohmic: $J(\omega) = \frac{\pi}{2}\alpha\omega_0^{1-s}\omega^s\Theta(\omega_c - \omega)$ and $0 < s < 1$:

$$\begin{array}{ll} \text{for } \omega_c^{-1} \ll t \ll T^{-1} & |\langle\sigma_+(t)\rangle| \approx e^{-\alpha(\omega_0 t)^{1-s}} \\ \text{for } t \gg T^{-1} & |\langle\sigma_+(t)\rangle| \approx e^{-\alpha T t (\omega_0 t)^{1-s}} \end{array}$$



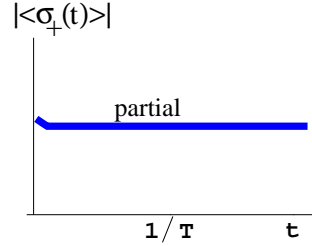
- Super-Ohmic: $J(\omega) = \frac{\pi}{2}\alpha\omega_0^{1-s}\omega^s\Theta(\omega_c - \omega)$ and $1 < s < 2$:

$$\begin{array}{ll} \text{for } \omega_c^{-1} \ll t \ll T^{-1} & |\langle\sigma_+(t)\rangle| \approx e^{-\alpha(\omega_c/\omega_0)^{s-1} t} \\ \text{for } t \gg T^{-1} & |\langle\sigma_+(t)\rangle| \approx e^{-\alpha T t (\omega_0 t)^{1-s}} \end{array}$$



- Soft gap: $J(\omega) = \frac{\pi}{2}\alpha\omega_0^{1-s}\omega^s\Theta(\omega_c - \omega)$ and $s > 2$:

$$\text{for } \omega_c^{-1} \ll t \quad |\langle\sigma_+(t)\rangle| \approx e^{-\alpha(\omega_c/\omega_0)^{s-1} t}$$



crossover in this case, i.e., $T^* = 0$. For $s \geq 2$ there is almost no additional decay.

The results obtained for different bath spectra are summarized in Table 1.

5. Preparation effects

In the previous section we considered specific initial conditions with a factorized density matrix. The bath was prepared in an equilibrium state characterized by temperature T , while the spin state was arbitrary. The state of the total system is, thus, a nonequilibrium one and dephasing is to be expected even at zero bath temperature. In this section we investigate what initial conditions may arise in real experiments.

The fully factorized initial state just described can in principle be prepared by the following Gedanken experiment: The spin is forced, e.g., by a strong external field, to be in a fixed state, say $|\uparrow\rangle$. The bath, which is kept coupled to the spin, relaxes to the equilibrium state of the Hamiltonian \mathcal{H}_\uparrow , e.g., at $T = 0$ to the ground state $|g_\uparrow\rangle$ of \mathcal{H}_\uparrow . Then, at $t = 0$, a *sudden* pulse of the external field is applied to change the spin state, e.g., to a superposition $\frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$. Since the bath has no time to respond, the resulting state is $|\text{i}\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle) \otimes |g_\uparrow\rangle$. Both components of this initial wave function now evolve in time according to the Hamiltonian (1). The first, $|\uparrow\rangle \otimes |g_\uparrow\rangle$, which is an eigenstate of (1), acquires only a trivial phase factor. The time evolution of the second component is more involved. Up to a phase factor it is given by $|\downarrow\rangle \otimes \exp(-i\mathcal{H}_\downarrow t/\hbar) |g_\uparrow\rangle$ where $\mathcal{H}_\downarrow \equiv \mathcal{H}_\text{b} - \sum_j c_j(a_j + a_j^\dagger)$. As the state $|g_\uparrow\rangle$ is not an eigenstate of \mathcal{H}_\downarrow , entanglement between the spin and the bath develops, and the coherence between the components of the spin's state is reduced by the factor $|\langle g_\uparrow | \exp(-i\mathcal{H}_\downarrow t/\hbar) |g_\uparrow\rangle| = |\langle g_0 | \exp(-i\Phi(t)) \exp(i\Phi) |g_0\rangle| = |P_{\omega_c}(t, T = 0)| < 1$. The function $P(t)$ was defined in Eq. (14). The subscript ω_c is added to indicate the value of the high-frequency cut-off of the bath which will play an important role in what follows.

In a real experiment of the type discussed the preparation pulse takes a finite time, τ_p . For instance, the $(\pi/2)_x$ -pulse which transforms the state $|\uparrow\rangle \rightarrow \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$, can be accomplished by putting $B_z = 0$ and $B_x = \hbar\omega_p$ for a time span $\tau_p = \pi/2\omega_p$. During this time the bath oscillators partially adjust to the changing spin state. The oscillators with (high) frequencies, $\omega_j \gg \omega_p$, follow the spin adiabatically. In contrast, the oscillators with low frequency, $\omega_j \ll \omega_p$, do not change their state. Assuming that the oscillators can be split into these two groups, we see that just after the $(\pi/2)_x$ -pulse the state of the system is $\frac{1}{\sqrt{2}}(|\uparrow\rangle \otimes |g_\uparrow^h\rangle + |\downarrow\rangle \otimes |g_\downarrow^h\rangle) \otimes |g_\uparrow^l\rangle$ where the superscripts 'h' and 'l' refer to high- and low-frequency oscillators, respectively. Thus, we arrive at an initial state with only the low-frequency oscillators factorized from the spin. For the off-diagonal element of the density matrix we obtain

$$|\langle\sigma_+(t)\rangle| = Z(\omega_c, \omega_p) |P_{\omega_p}(t)|, \quad (17)$$

where $Z(\omega_c, \omega_p) \equiv |\langle g_\uparrow^h | g_\downarrow^h \rangle|$ and $P_{\omega_p}(t)$ is given by the same expressions as before, except that the high-frequency cut-off is reduced to ω_p .

The high frequency oscillators still contribute to the reduction of $|\langle \sigma_+(t) \rangle|$ – via the factor $Z(\omega_c, \omega_p)$ – however, this effect is reversible. To illustrate this we consider the following continuation of the experiment. After the $(\pi/2)$ pulse we allow for a free evolution of the system during time t with magnetic field $B_z = \Delta E$ along z axis. Then we apply a $(-\pi/2)$ pulse and measure σ_z . Without dissipation the result would be $\langle \sigma_z \rangle = \cos(\Delta E t)$. With dissipation the state of the system after time t is

$$\frac{1}{\sqrt{2}} \left(e^{i\Delta E t/2} |\uparrow\rangle \otimes |g_\uparrow^h\rangle \otimes |g_\uparrow^l\rangle + e^{-i\Delta E t/2} |\downarrow\rangle \otimes |g_\downarrow^h\rangle \otimes e^{-i\mathcal{H}_\downarrow t/\hbar} |g_\uparrow^l\rangle \right). \quad (18)$$

After the $(-\pi/2)$ pulse (also of width $\pi/2\omega_p$) we obtain the following state:

$$\begin{aligned} & \frac{1}{2} |\uparrow\rangle \otimes |g_\uparrow^h\rangle \otimes \left(e^{i\Delta E t/2} |g_\uparrow^l\rangle + e^{-i\Delta E t/2} e^{-i\mathcal{H}_\downarrow t/\hbar} |g_\uparrow^l\rangle \right) + \\ & \frac{1}{2} |\downarrow\rangle \otimes |g_\downarrow^h\rangle \otimes \left(-e^{i\Delta E t/2} |g_\uparrow^l\rangle + e^{-i\Delta E t/2} e^{-i\mathcal{H}_\downarrow t/\hbar} |g_\uparrow^l\rangle \right). \end{aligned} \quad (19)$$

From this we finally get $\langle \sigma_z \rangle = \text{Re} [P_{\omega_p}(t) e^{-i\Delta E t}]$. Thus the amplitude of the coherent oscillations of σ_z is reduced only by the factor $|P_{\omega_p}(t)|$ associated with slow oscillators. The high frequency factor $Z(\omega_c, \omega_p)$ does not appear. To interpret this result we note that we could have discussed the experiment in terms of renormalized spins $|\tilde{\uparrow}\rangle \equiv |\uparrow\rangle |g_\uparrow^h\rangle$ and $|\tilde{\downarrow}\rangle \equiv |\downarrow\rangle |g_\downarrow^h\rangle$, and assuming that the high frequency cutoff of the bath is ω_p .

It is interesting to compare further the two scenarios with instantaneous and finite-time preparation further. The time evolution after the instantaneous preparation is governed by $P_{\omega_c}(t)$. For $T \ll \omega_p$ and $t \gg 1/\omega_p$ and arbitrary spectral density $J(\omega)$ it satisfies the following relation: $P_{\omega_c}(t) = Z^2(\omega_c, \omega_p) P_{\omega_p}(t)$, which follows from $\langle g_\uparrow^h | \exp(-i\mathcal{H}_\downarrow t/\hbar) | g_\uparrow^h \rangle \rightarrow |\langle g_\uparrow^h | g_\downarrow^h \rangle|^2$ for $t \gg 1/\omega_p$. Thus for the instantaneous preparation the reduction due to the high frequency oscillators is equal to $Z^2(\omega_c, \omega_p)$, while a look at the finite-time preparation result (17) shows that in this case the reduction is weaker, given by a single power of $Z(\omega_c, \omega_p)$ only. Moreover, in the slow preparation experiment the factor $Z(\omega_c, \omega_p)$ originates from the overlap of two ‘simple’ wave functions, $|g_\uparrow^h\rangle$ and $|g_\downarrow^h\rangle$, which can be further adiabatically manipulated, as described above, and this reduction can be recovered. This effect is to be interpreted as a renormalization. On the other hand, for the instantaneous preparation the high frequency contribution to the dephasing originates from the overlap of the states $|g_\uparrow^h\rangle$ and $e^{-i\mathcal{H}_\downarrow t/\hbar} |g_\uparrow^h\rangle$. The latter is a complicated excited state of the bath with many nonzero

amplitudes evolving with different frequencies. There is no simple (macroscopic) way to reverse the dephasing associated with this state. Thus we observe that the time scale of the manipulating pulses determines the border between the oscillators responsible for dephasing and the oscillators responsible for renormalization.

6. Response functions

In the limit $\theta = 0$ we can also calculate exactly the linear response of $\tau_x = \sigma_x$ to a weak magnetic field in the x -direction, $B_x(t)$:

$$\chi_{xx}(t) = \frac{i}{\hbar} \Theta(t) \langle \tau_x(t) \tau_x(0) - \tau_x(0) \tau_x(t) \rangle . \quad (20)$$

Using the equilibrium density matrix

$$\hat{\rho}^{\text{eq}} = (1 + e^{-\beta \Delta E})^{-1} \left[|\uparrow\rangle \langle \uparrow| \otimes \hat{\rho}_{\uparrow} + e^{-\beta \Delta E} |\downarrow\rangle \langle \downarrow| \otimes \hat{\rho}_{\downarrow} \right] , \quad (21)$$

where $\hat{\rho}_{\uparrow} \propto \exp(-\beta \mathcal{H}_{\uparrow})$ is the bath density matrix adjusted to the spin state $|\uparrow\rangle$, and similar for $\hat{\rho}_{\downarrow}$, we obtain the susceptibility

$$\chi_{xx}(t) = -\frac{2\hbar^{-1}\Theta(t)}{1 + e^{-\beta \Delta E}} \text{Im} \left[P_{\omega_c}(t) e^{-i\Delta E t} + e^{-\beta \Delta E} P_{\omega_c}(t) e^{i\Delta E t} \right] . \quad (22)$$

Thus, to calculate the response function one has to use the full factor $P_{\omega_c}(t)$, corresponding to the instantaneous preparation of an initial state. This can be understood by looking at the Kubo formula (20). The operator $\tau_x(0)$ flips only the bare spin without touching the oscillators, as if an infinitely sharp ($\pi/2$) pulse was applied.

The imaginary part of the Fourier transform of $\chi(t)$, which describes dissipation, is

$$\chi''_{xx}(\omega) = \frac{1}{2(1 + e^{-\beta \Delta E})} \left[P(\hbar\omega - \Delta E) + e^{-\beta \Delta E} P(\hbar\omega + \Delta E) \right] - \dots(-\omega) . \quad (23)$$

At $T = 0$ and positive values of ω we use the expression for $P(E)$ from Ref. [1] to obtain

$$\chi''_{xx}(\omega) = \frac{1}{2} P(\hbar\omega - \Delta E) = \Theta(\hbar\omega - \Delta E) \frac{e^{-2\gamma\alpha} (\hbar\omega_c)^{-2\alpha}}{2\Gamma(2\alpha)} (\hbar\omega - \Delta E)^{2\alpha-1} . \quad (24)$$

We observe that the dissipative part χ''_{xx} has a gap ΔE , which corresponds to the minimal energy needed to flip the spin, and a power-law behavior as ω approaches the threshold. This behavior of $\chi''_{xx}(\omega)$ is known from the

orthogonality catastrophe scenario [5]. It implies that the ground state of the oscillator bath for different spin states, $|g_\uparrow\rangle$ and $|g_\downarrow\rangle$, are *macroscopically* orthogonal. In particular, for an Ohmic bath we recover the behavior typical for the problem of X-ray absorption in metals [5].

As $\chi''(\omega)$ characterizes the dissipation in the system (absorption of energy from the perturbing magnetic field) it is interesting to understand the respective roles of high- and low-frequency oscillators. We use the spectral decomposition for χ'' at $T = 0$,

$$\chi''(\omega) = \pi \sum_n |\langle 0 | \tau_x | n \rangle|^2 [\delta(\omega - E_n) - \delta(\omega + E_n)] , \quad (25)$$

where n denotes exact eigenstates of the system. These are $|\uparrow\rangle |n_\uparrow\rangle$ and $|\downarrow\rangle |n_\downarrow\rangle$, where $|n_\uparrow\rangle$ and $|n_\downarrow\rangle$ denote the excited (multi-oscillator) states of the Hamiltonians \mathcal{H}_\uparrow and \mathcal{H}_\downarrow . The ground state is $|\uparrow\rangle |g_\uparrow\rangle$ and the only excited states that contribute to $\chi''(\omega)$ are $|\downarrow\rangle |n_\downarrow\rangle$ with $\mathcal{H}_\downarrow |n_\downarrow\rangle = (\omega - \Delta E) |n_\downarrow\rangle$. This means that all the oscillators with frequencies $\omega_j > \omega - \Delta E$ have to be in the ground state. Therefore we obtain for $\omega_p > \omega - \Delta E$

$$\chi''_{\omega_c}(\omega) = Z^2(\omega_c, \omega_p) \chi''_{\omega_p}(\omega) . \quad (26)$$

To interpret this result we generalize the coupling to the magnetic field by introducing a g factor: $H_{\text{int}} = -(g/2)\delta B_x(t)\sigma_x$. Then, if the applied magnetic field can be independently measured, the observable quantity corresponding, e.g., to the energy absorption is

$$\chi_{xx}(t) = g^2 \frac{i}{\hbar} \Theta(t) \langle [\sigma_x(t), \sigma_x(0)] \rangle . \quad (27)$$

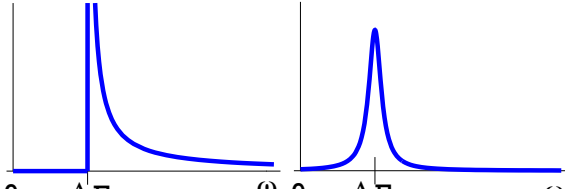
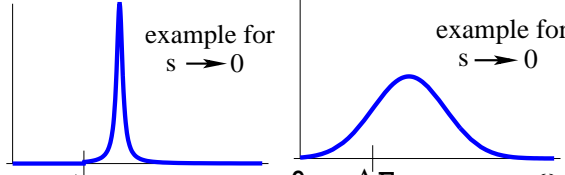
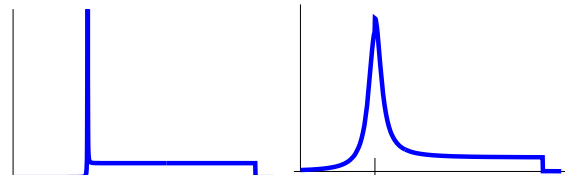
Thus, Eq. (26) tells us that by measuring the response of the spin at frequencies $\omega < \omega_p + \Delta E$ we cannot distinguish between a model with upper cutoff ω_c and $g = 1$ and a model with cutoff ω_p and $g = Z(\omega_c, \omega_p)$. This is the usual situation in the renormalization group context. Thus, again, we note that high-frequency oscillators are naturally associated with renormalization effects.

We collect the results for χ'' for various spectra in Table 2. The results are shown for temperatures lower and higher than the crossover temperature introduced in Section 4.

7. Summary

The examples presented above show that for a quantum two-state system with a non-equilibrium initial state, described by a factorized initial density matrix, dephasing persists down to zero bath temperature. An Ohmic

TABLE 2. Response functions for different bath spectra.

Bath spectrum $J(\omega) = \frac{\pi}{2} \alpha \omega_0^{1-s} \omega^s$ $\times \Theta(\omega_c - \omega)$	Response function $\chi_{xx}(t) = i\Theta(t)\langle[\sigma_x(t), \sigma_x(0)]\rangle$ $\chi''_{xx}(\omega), T < T^*$ $\chi''_{xx}(\omega), T > T^*$
Ohmic $s = 1$	 <div style="display: flex; justify-content: space-around; margin-top: 5px;"> <div data-bbox="516 714 779 772"> $\frac{\alpha \Theta(\omega - \Delta E)}{(\omega - \Delta E)^{(1-2\alpha)}}$ </div> <div data-bbox="795 714 1078 772"> $\frac{\alpha T}{(\alpha T)^2 + (\omega - \Delta E)^2}$ </div> </div>
Sub-Ohmic $0 \leq s < 1$	 <div style="display: flex; justify-content: space-around; margin-top: 5px;"> <div data-bbox="516 1029 779 1094"> $\frac{\alpha \omega_0 \theta(\omega - \Delta E)}{(\alpha \omega_0)^2 + (\omega - \Delta E - \alpha \omega_0 \ln(\dots))^2}$ </div> <div data-bbox="795 1029 1078 1094"> $\exp \left[-\frac{(\omega - \Delta E - \alpha \omega_0 \ln(\dots))^2}{\alpha \omega_0 T \ln(\dots)} \right]$ </div> </div>
Super-Ohmic $1 < s \leq 2$	 <div style="display: flex; justify-content: space-around; margin-top: 5px;"> <div data-bbox="516 1344 779 1415"> $Z^2 \delta(\omega - \Delta E) + \dots$ </div> <div data-bbox="795 1344 1078 1415"> $Z^2 \delta_{\Gamma_\varphi}(\omega - \Delta E) + \dots$ </div> </div>

environment leads to a power-law dephasing at $T = 0$, while a sub-Ohmic bath yields exponential dephasing. The reason is that the factorized initial state, even with the bath in the ground state of the bath Hamiltonian, is actually a superposition of many excited states of the total coupled system. In a real experiment only a part of the environment, the oscillators with low frequencies, can be prepared factorized from the two level system. These oscillators still lead to dephasing, whereas the high-frequency oscillators lead

to renormalization effects. The examples demonstrate that experimental conditions, e.g., details of the system's initial state preparation, determine which part of the environment contributes to dephasing and which part leads to renormalization. The finite preparation time $\sim 1/\omega_p$ also introduces a natural high-frequency cutoff in the description of dephasing effects. We have further demonstrated that dephasing and renormalization effects influence the response functions of the two level system. We noted that they exhibit features known for the orthogonality catastrophe, including a power-law divergence above a threshold.

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